# References

Aggarwal, A. and C. A. Floudas (1990). Synthesis of General Distillation Sequences - Nonsharp Separations. *Computers Chem. Engng.* **14**(6), 631–653.

Agrawal, R. (1996). Synthesis of Distillation Column Configurations for a Multicomponent Separation. *Ind. Eng. Chem. Res.* **35**, 1059–1071.

Agrawal, R. (2000*a*). A Method to Draw Fully Thermally Coupled Distillation Column Configurations for Multicomponent Distillation. *Trans IChemE Part A* **78**, 454–464.

Agrawal, R. (2000*b*). Thermally Coupled Distillation with Reduced Number of Intercolumn Vapor Transfers. *AIChE J.* **46**(11), 2198–2210.

Agrawal, R. (2003). Synthesis of Multicomponent Distillation Column Configurations. *AIChE J.* **49**(2), 379–401.

Agrawal, R. and Z. T. Fidkowski (1998). Are Thermally Coupled Distillation Columns Always Thermodynamically More Efficient for Ternary Distillations?. *Ind. Eng. Chem. Res.* **37**(8), 3444–3454.

Agrawal, R. and Z. T. Fidkowski (1999a). New Thermally Coupled Schemes for Ternary Distillation. *AIChE J.* **45**, 485–496.

Andrecovich, M. J. and A. W. Westerberg (1985*aa*). An MILP Formulation for Heat-Integrated Distillation Sequence Synthesis. *AIChE J.* **31**(9), 1461–1474.

Andrecovich, M. J. and A. W. Westerberg (1985*ab*). A Simple Synthesis Method Based on Utility Bounding for Heat-Integrated Distillation Sequences. *AIChE J.* **31**(9), 363–375.

Annakou, O. and P. Mizsey (1996). Rigorous Comparative Study of Energy-Integrated Distillation Schemes. *AIChE J.* **35**(6), 1877–1885.

Balas, E. (1985). Disjunctive Programming and a Hierarchy of Relaxations for Discrete Optimization Problems. *SIAM J. Alg. Discrete Methods* **6**, 466–486.

Beale, E. M. L. (1977). *Integer Programming. In D. A. H. Jacobs, editor,* The State of The Art in Numerical Analysis*, pages 409-448*. Academic Press. London.

Bek-Pedersen, E. (2003). Synthesis and Design of Distillation Based Separation Schemes. PhD dissertation. Technical University of Denmark.

Benallou, A., D. E. Seborg and D. A. Mellichamp (1982). Low Order, Physically Lumped Dynamic Models for Distillation Column Control. *AIChE Annual Meeting, Los Angeles, Paper 9e*.

Biegler, L. T., I. E. Grossmann and A. W. Westerberg (1997). *Systematic Methods of Chemical Process Design*. Prentice Hall PTR. New Jersey.

Brooke, A., D. Kendrik and A. Meeraus (1988). *GAMS: A User's Guide*. Scientific Press. Palo Alto, CA.

Caballero, J. A. and I. E. Grossmann (1999). Aggregated Models for Integrated Distillation Systems. *Ind. Eng. Chem. Res.* **38**, 2330–2344.

Caballero, J. A. and I. E. Grossmann (2001). Generalized Disjunctive Programming Model for the Optimal Synthesis of Thermally Linked Distillation Columns. *Ind. Eng. Chem. Res.* **40**, 2260–2274.

CAPEC, Department of Chemical Engineering DTU (1999). *ICAS Users Manual*. Lyngby, Denmark.

Carlberg, N. A. and A. W. Westerberg (1989*a*). Temperature-Heat Diagrams for Complex Columns. 2. Underwood's Method for Side Strippers and Enrichers. *Ind. Eng. Chem. Res.* **28**, 1379–1386.

Carlberg, N. A. and A. W. Westerberg (1989*b*). Temperature-Heat Diagrams for Complex Columns. 3. Underwood's Method for the Petlyuk Configuration. *Ind. Eng. Chem. Res.* **28**, 1386–1397.

Cerda, J., A. W. Westerberg, D. Mason and B. Linnhoff (1983). Minimum Utility Usage in Heat Exchanger Network Synthesis-A Transportation Problem. *Chem. Eng. Science* **38**(3), 373–383.

Chang, C.T., K.K. Chu and J.R. Hwang (1994). Application of the Generalized Stream Structure in HEN Synthesis. *Comp. Chem. Engng.* **18**, 345.

Chavez, R. C., J. D. Seader and T. L. Wayburn (1986). Multiple Steady State Solutions for Interlinked Separation Systems. *Ind. Eng. Chem. Fundam.* **25**, 566–576.

Cho, Y. S. and B. Joseph (1983*a*). Reduced-Order Steady-State and Dynamic Models for Separation Processes. *AIChE J.* **29**(2), 261–269.

Cho, Y. S. and B. Joseph (1983*b*). Reduced-Order Steady-State and Dynamic Models for Separation Processes - Part II. Application to Nonlinear Multicomponent Systems. *AIChE J.* **29**(2), 270–276.

Cho, Y. S. and B. Joseph (1984). Reduced-Order Steady-State and Dynamic Models for Separation Processes - Part III. Application to Columns with Multiple Feeds and Sidestreams. *Comput. Chem. Engng.* **8**(2), 81–90.

Ciric, A. R. and D. Gu (1994*a*). Synthesis of Nonequilibrium Reactive Distillation Processes by MINLP OPtimization. *AIChE J.* **40**(9), 1479–1487.

Ciric, A.R. and Deyao Gu (1994*b*). Synthesis of Nonequilibrium Reactive Distillation Processes by MINLP Optimization. *AIChE Jl.* **40**, 1479.

Ciric, A.R. and P. Miao (1994). Steady State Multiplicities in an Ethylene Glycol Reactive Distillation Column. *Ind. Eng. Chem. Res.* **33**, 2738.

Ciric, A.R. and T. Jia (1991). Economic Sensitivity Analysis of Waste Treatment Cost in Source Reduction Projects: Continuous Optimization Problems. *AIChE Annual Meeting.*

Clocksin, W.F. and C.S. Mellish (1981). *Programming in Prolog*. Springer-Verlag. New York.

Doherty, M. F. and M. F. Malone (2001). *Conceptual Design of Distillation Systems*. McGraw-Hill Co, Inc.. New York.

Douglas, J. M. (1988). *Conceptual Design of Chemical Processes*. McGraw Hill. New York.

Drud, A. S. (1995). *A System for Large Scale Nonlinear Optimization - Reference Manual*. ARKI Consulting and Development A/S. Bagsvaerd, Denmark.

Dunnebier, G. and C. C. Pantelides (1999). Optimal Design of Thermally Coupled Distillation Columns. *Ind. Eng. Chem. Res.* **38**, 162–176.

Duran, M. A. and I. E. Grossmann (1986*a*). An Outer Approximation Algorithm for a Class of Mixed Integer Nonlinear Problems. *Mathematical Programming* **36**, 307–339.

Duran, M. A. and I. E. Grossmann (1986*b*). Simultaneous Optimization and Heat Integration of Chemical Processes. *AIChE J.* **32**, 123–138.

El-Halwalgi, M. M. and V. Manousiouthakis (1989). Synthesis of Mass Exchange Networks. *AIChE J.* **35**(8), 1233–1244.

Eliceche, A. M. and R. W. H. Sargent (1981). Synthesis and Design of Distillation Systems. *IChemE Symp Ser* **61**, 1–22.

Fidkowski, Z. T. and L. Krolikowski (1986). Thermally Coupled System of Distillation Columns: Optimisation Procedure. *AIChE J.* **32**, 537–546.

Floudas, C. A. (1987). Separation Synthesis of Multicomponent Feed Streams into Multicomponent Product Streams. *AIChE J.* **33**(4), 540–550.

Floudas, C. A. (1995). *Nonlinear and Mixed-Integer Optimization*. Oxford University Press. New York.

Floudas, C. A. and S. H. Anastasiadis (1988). Synthesis of Distillation Sequences With Several Multicomponent Feed and Product Streams. *Chem. Eng. Science* **43**(9), 2407–2419.

Fraga, E. S. and K. I. M. McKinnon (1995). Portable Code for Process Synthesis Using Workstation Clusters and Distributed Memory Multicomputers. *Comput. Chem. Eng.* **19**, 759–773.

Freshwater, D.C. and B.D. Henry (1975). The Optimal Configuration of Multicomponent Distillation Trains. *Chem. Eng.* **301**, 533–536.

Geoffrion, A. M. (1972). Generalized Benders Decomposition. *Journal of Optimization Theory and Applications* **10**, 237–260.

Georgakis, C. and M. A. Stoever (1982). Time Domain Order Reduction of Tridiagonal Dynamics of Staged Processes - I. Uniform Lumping. *Chem. Eng. Science* **37**, 687–697.

Glinos, K. and F. Malone (1988). Optimality Regions for Complex Column Alternatives in Distillation Systems. *Chem. Eng. Res. Des.* **66**, 229–240.

Grossmann, I. E. (1985). Mixed-Integer Programming Approach for the Synthesis of Integrated Process Flowsheets. *Computers Chem. Engng.* **9**, 463–482.

Grossmann, I. E., H. Yeomans and Z. Kravanja (1998). A Rigorous Disjunctive Optimization Model for Simultaneous Flowsheet Optimization and Heat Integration. *Computers Chem. Engng.* **22**, S157–S164.

Hendry, J. E. and R. R. Hughes (1972). Generating Separation Process Flowsheets. *Chem. Eng. Prog.* **68**, 71–76.

Hohmann, E. C., M. T. Sander and M. T. Dunford (1982). A New Approach to the Synthesis of Multicomponent Separation Schemes. *Chem. Eng. Commun.* **17**, 273–284.

Hostrup, M., R. Gani, Z. Kravanja, A. Sorsak and I. E. Grossmann (2001). Integration of Thermodynamic Insights and MINLP Optimization for the Synthesis, Design and Analysis of Process Flowsheets. *Computers Chem. Engng.* **25**, 73–83.

Huss, R. S. and A. W. Westerberg (1996*a*). Collocation Methods for Distillation Design. 1. Model Description and Testing. *Ind. Eng. Chem. Res.* **35**, 1603–1610.

Huss, R. S. and A. W. Westerberg (1996*b*). Collocation Methods for Distillation Design. 2. Applications for Distillation. *Ind. Eng. Chem. Res.* **35**, 1611–1623.

Ismail, S. R. (1998). A Generalised Modular Framework for the Synthesis of Nonideal Separation and Reactive Separation Processes. PhD dissertation. Imperial College of Science, Technology and Medicine, London.

Ismail, S. R., E. N. Pistikopoulos and K. P. Papalexandri (1999). Modular Representation Synthesis Framework for Homogeneous Azeotropic Separation. *AIChE J.* **45**(8), 1701–1720.

Ismail, S. R., P. Proios and E. N. Pistikopoulos (2001). Modular Synthesis Framework for Combined Separation/Reactive Systems. *AIChE J.* **47**(3), 629–650.

Jaksland, C., Gani R. and Lien K. (1995). Separation Process Design and Synthesis Based on Thermodynamic Insights. *Chem. Eng. Science* **50**, 511–530.

Kakhu, A. I. and J. R. Flower (1988). Synthesising Heat-Integrated Distillation Sequences Using Mixed Integer Programming. *Chem. Eng. Res. Des.* **66**, 241–254.

Kocis, G. R. and I. E. Grossmann (1989). Computational Experience with DICOPT Solving MINLP Problems in Process Systems Engineering. *Computers Chem. Engng.* **13**, 307–315.

Kokossis, A.C. and C.A. Floudas (1991). Synthesis of Isothermal Reactor-Separator-Recycle Systems. *Chem. Eng. Sci.* **46**, 1361.

Kravanja, Z. and I. E. Grossmann (1993). PROSYN-An Automated Topology and Parameter Process Synthesizer. *Comput. Chem. Engng.* **17**, S87–S94.

Kravanja, Z. and I. E. Grossmann (1994). New Developments and Capabilities in PROSYN-An Automated Topology and Parameter Process Synthesizer. *Comput. Chem. Engng.* **18**, 1097–1114.

Linnhoff, B., H. Dunford and R. Smith (1983). Heat integration of distillation columns into overall processes. *Chem. Eng. Science* **35**, 1175–1188.

Luyben, M.L. and W.L. Luyben (1995). Design and Control of a Complex Process Involving Two Reaction Steps, Three Distillation Columns, and Two Recycle Streams. *Ind. Eng. Chem. Res.* **34**(11), 3885 – 3898.

Mei, Ding (1995). An SQP Based MINLP Algorithm and its Apllication to Synthesis of Distillation Systems. PhD dissertation. Imperial College of Science, Technology and Medicine, London.

Mix, T. W., J. S. Dweck, M. Weiberg and R. C. Armstrong (1978). Energy Conservation in Distillation. *Chem. Eng. Prog.* **74**(4), 49–55.

Morari, M. and C. Faith (1980). The Synthesis of Distillation Trains with Heat Integration. *AIChE J.* **26**, 916–928.

Nishida, N., G. Stephanopoulos and A.W. Westerberg (1981). A Review of Process Synthesis. *AIChE Jl.* **27**, 321.

Novak, Z., Z. Kravanja and I. E. Grossmann (1996). Simultaneous Synthesis of Distillation Sequences in Overall Process Schemes Using an Improved MINLP Approach. *Comput. Chem. Engng.* **20**, 1425–1440.

Papalexandri, K. P. and E. N. Pistikopoulos (1996). Generalized Modular Representation Framework for Process Synthesis. *AIChE J.* **42**(4), 1010–1032.

Papalexandri, K. P., E. N. Pistikopoulos and C. A. Floudas (1995). Mass Exchange Networks for Waste Minimization: A Simultaneous Approach. *Trans IChemE Part A* **72**, 279–294.

Papalexandri, K.P. (1996). Flexibility and Controlability in the Synthesis of Mass/Heat Integrated Process Systems. PhD dissertation. Imperial College of Science, Technology and Medicine, London, UK.

Papoulias, S. and I. E. Grossmann (1983). A Structural Optimization Approach in Process Synthesis. I: Utility Systems, II: Heat Recovery Networks, III: Total Processing Systems. *Computers Chem. Engng.* **7**(6), 695–734.

Paterson, W.R. (1984). A replacement for the Logarithmic Mean. *Chem. Eng. Science* **39**, 1635 – 1636.

Paules, G. E. and C. A. Floudas (1988). A Mixed Integer Nonlinear Programming Formulation for the Synthesis of Heat Integrated Distillation Sequences. *Computers Chem. Engng.* **12**(6), 531–546.

Paules, G. E. and C. A. Floudas (1989). APROS: Algorithmic Development Methodology For Discrete-Continuous Optimization Problems. *Operations Research* **37**(6), 902–915.

Proios, P. (1999). Generalized Modular Representation of the Petlyuk/Dividing Wall Column. M.Sc. dissertation. Imperial College of Science, Technology and Medicine, London.

Proios, P. (2004). Generalized Modular Framework for Distillation Column Synthesis. PhD thesis. Imperial College of Science, Technology and Medicine, London, UK.

Raman, R. and I. E. Grossmann (1991). Relation Between MILP Modeling and Logical Inference for Chemical Process Synthesis. *Comput. Chem. Engng.* **15**(2), 73–84.

Raman, R. and I. E. Grossmann (1993). Symbolic Integration of Logic in Mixed Integer Linear Programming Techniques for Process Synthesis. *Computers Chem. Engng.* **17**, 909–927.

Raman, R. and I. E. Grossmann (1994). Modelling and Computational Techniques for Logic Based Integer Programming. *Comput. Chem. Engng.* **18**(7), 563–578.

Rathore, R., K. van Wormer and G. Powers (1974). Synthesis Strategies for Multicomponent Separation Systems with Energy Integration. *AIChE J.* **20**, 491–502.

Reid, R. C. (1987). *The Properties of Gases and Liquids*. 4th ed.. McGraw-Hill.

Rigg, T.J. and R.E. Swaney (1994). Synthesis of General Equilibrium-based Separation Processes Using a Network Flow Model. *Proceedings of PSE'94* p. 55.

Sargent, R. W. H. (1998). A Functional Approach to Process Synthesis and its Application to Distillation Systems. *Comput. Chem. Engng.* **22**(1-2), 31–45.

Sargent, R. W. H. and K. Gaminibandara (1976). *Optimal Design of Plate Distillation Columns,* Optimization in Action. Academic Press. London.

Seader, J. D. and A. W. Westerberg (1977). A Combined Heuristic and Evolutionary Strategy for Synthesis of Simple Separation Sequences. *AIChE J.* **23**, 951–954.

Seferlis, P. and A.N. Hrymak (1994*a*). Optimization of Distillation Units Using Collocation Models. *AIChE J.* **40**(5), 813–825.

Seferlis, P. and A.N. Hrymak (1994*b*). Adaptive Collocation on Finite Elements Models for the Optimization of Multistage Distillation Units. *Chem. Eng. Science* **49**(9), 1369–1382.

Smith, E. M. (1996). On the Optimal Design of Continuous Processes. PhD dissertation. Imperial College of Science, Technology and Medicine, London.

Smith, E. M. B. and C. C. Pantelides (1995). Design of Reaction/Separation Networks Using Detailed Models. *Computers Chem. Engng.* **19**, S83–S88.

Sophos, A., G. Stephanopoulos and M. Morari (1978). Synthesis of optimum distillation sequences with heat integration schemes. Paper 42d. 71st Annl AIChE Mtg. Miami, Florida.

Sorel, E. (1889). Sur la Rectification de l' Alcohol. *Comptes Rendus* **CVIII**, 1128.

Stephanopoulos, G. and A. W. Westerberg (1976). Studies in Process Synthesis, II:Evolutionary Synthesis of Optimal Process Flowsheets. *Chem. Eng. Science* **31**, 195–204.

Stewart, W.E., K.L. Levien and M. Morari (1985). Simulation Of Fractionation By Orthogonal Collocation. *Chem. Eng. Science* **40**(3), 409–421.

Swartz, C.L.E. and W.E. Stewart (1986). A Collocation Approach to Distillation Column Design. *AIChE J.* **32**(11), 1832–1838.

Swartz, C.L.E. and W.E. Stewart (1987). Finite-Element Steady State Simulation of Multiphase Distillation. *AIChE J.* **33**, 1977–1985.

Tedder, D. W. and D. F. Rudd (1978). Parametric Studies in Industrial Distillation: Part 1. Design Comparisons. *AIChE J.* **24**(2), 303–315.

Thompson, R. W. and C. J. King (1972). Systematic Synthesis of Separation Schemes. *AIChE J.* **18**, 941–948.

Triantafyllou, C. and R. Smith (1992). The Design and Optimisation of Fully Thermally Coupled Distillation Columns. *Trans. Inst. Chem.* **70**, 118–132.

Van Dongen, D. B. and M. F. Doherty (1985). Design and Synthesis of Homogeneous Azeotropic Distillations. 1. Problem Formulation for a Single Column. *Ind. Eng. Chem. Fundam.* **24**, 454–463.

Viswanathan, J. and I. E. Grossmann (1990). A Combined Penalty Function and Outer-Approximation Method for MINLP Optimization. *Comput. Chem. Engng.* **14**(7), 769–782.

Viswanathan, J. and I. E. Grossmann (1993). Optimal Feed Locations and Number of Trays for Distillation Columns with Multiple Feeds. *Ind. Eng. Chem. Res.* **32**, 2942–2949.

Wahl, E. F. and P. Marriott (1970). Understanding and Predictions of the Dynamic Behaviour of Distillation Columns. *Ind. Engng. Chem. Proc. Des. Dev.* **9**, 396–407.

Wehe, R. R. and A. W. Westerberg (1987). An Algorithmic Procedure for the Synthesis of Distillation Sequences with Bypass. *Computers Chem. Engng.* **11**(6), 619–627.

Westerberg, A. W. and M. J. Andrecovich (1985*b*). Utility Bounds for Nonconstant Q Delta T for Heat-Integrated Distillation Sequence Synthesis. *AIChE J.* **31**(9), 1461–1474.

Yee, T. F. and I. E. Grossmann (1990). Simultaneous Optimization Models for Heat Integration - III. Heat Exchanger Network Synthesis. *Comput. Chem. Engng.* **14**, 1165–1184.

Yee, T. F., I. E. Grossmann and Z. Kravanja (1990). Simultaneous Optimization Models for Heat Integration - I. Area and Energy Targeting and Modelling of Multistream Exchangers. *Comput. Chem. Engng.* **14**, 1151–1164.

Yeomans, H. and I. E. Grossmann (1999*a*). A Systematic Modelling Framework of Superstructure Optimization in Process Synthesis. *Computers Chem. Engng.* **23**, 709–731.

Yeomans, H. and I. E. Grossmann (1999*b*). Nonlinear Disjunctive Programming Models for the Synthesis of Heat Integrated Distillation Sequences. *Computers Chem. Engng.* **23**, 1135–1151.

Yeomans, H. and I. E. Grossmann (2000*a*). Disjunctive Programming Models for the Optimal Design of Distillation Columns and Separation Sequences. *Ind. Eng. Chem. Res.* **39**, 1637–1648.

Yeomans, H. and I. E. Grossmann (2000*b*). Optimal Design of Complex Distillation Columns Using Rigorous Tray-by-Tray Disjunctive Programming Models. *Ind. Eng. Chem. Res.* **39**, 4326–4335.

Zhang, L. and A. A. Linninger (2004). A Temperature Collocation Algorithm for Fast and Robust Distillation Design. *Ind. Eng. Chem. Res. (submitted for publication).*